Truncated many-body dynamics of interacting bosons: A variational principle with error monitoring

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Abstract

We introduce a scheme to describe the evolution of an interacting system of bosons, for which the field operator expansion is truncated after a finite number of modes, in a rigourously controlled manner. Using McLachlan's principle of least error, we find a self-consistent set of equations for the many-body state. As a particular benefit, and in distinction to previously proposed approaches, our approach allows for the dynamical increase of the number of orbitals during the temporal evolution. The additional orbitals, determined by the condition of least error of the truncated evolution relative to the exact one, are obtained from an initial trial state by a method we call steepest constrained descent.

Contents

1. Introduction

When we treat an atom, such as ^{87}Rb, ^{23}Na, and ^{7}Li which consists of an even number of fermions, as a whole, the Fock space creation and annihilation

operators of these composites satisfy bosonic commutation relations. Since the experimental realization of Bose-Einstein condensates [1], a large variety of experiments with these bosonic isotopes have opened up a fascinating mesoscopic and macroscopic quantum world [2]. After an initial period, concentrating on the effective single-particle physics of these ultracold dilute gases [3], more recently their many-body physics came into focus, revealing rich and hitherto unexpected possibilities to test fundamental correlation properties at the microscopic level [4].

The extension to a true many-body physics, incorporating quantum correlations beyond mean-field, requires, however, vast computational resources when both the number of particles and the interaction between those particles increases. Therefore, a simplification of the problem by *truncating* the field operator expansion to a finite number of modes (or, as an equivalent term, single-particle orbitals) has been commonly utilized to obtain results relevant to the prediction of experiments in trapped bosonic quantum gases. The most extreme truncation, the semiclassical form of mean-field theory, retaining just one orbital, gives the well-known Gross-Pitaevskiĭ equation. Without the aid of contemporary computers, it seemed to be inevitable until most recently, particularly in out-of-equilibrium situations far away from the ground state, to reduce the complexity of the problem at hand as much as possible, and hence to use the Gross-Pitaevskiĭ equation approach. With the increased interest in many-body physics, however, there arose the necessity to go beyond the all-too-simplified mean field approach of the Gross-Pitaevskiĭ equation. The accuracy of predictions on many-body correlations and the corresponding response functions will obviously increase with a less severe degree of truncation, though the solutions will not be exact still.

To derive the equations of many-body evolution, various variational approaches can be employed. Historically the first was the variational ansatz of Dirac and Frenkel [5, 6], followed by McLachlan's variational principle [7] and the time-dependent variational principle (TDVP), which is a principle of stationary action [8, 9]. Therefore, there are various, not necessarily equivalent, choices of variational principle for finding the equation of motion of the truncated many-body evolution. The Dirac-Frenkel principle imposes $\langle \delta\Phi | \hat{H} - i\partial_t | \Phi \rangle = 0$ ($\hbar \equiv 1$), where $\delta\Phi$ denotes any possible variations of the many-body state Φ with respect to a given set of variational parameters, whereas McLachlan's principle requires that the error of many-body evolution must be minimized. On the other hand, the TDVP, as stated, requires stationarity of a given action. The three principles thus support quite different doctrines.

Applying either the TDVP or the Dirac-Frenkel's principle, the authors in [9] have proposed a method they called MCTDHB (Multi-Configurational Time-Dependent Hartree method for Bosons). This approach has, for example, provided tools for the description of the fragmentation of bosonic many-body states [10, 11, 12, 13]. We will describe below in detail that, besides its many beneficial properties, the MCTDHB method is incomplete in certain situations. Specifically, when the single-particle density matrix (SPDM) becomes singular, i.e. noninvertible, the method fails. As a consequence, MCTDHB does not provide a way to propagate, for example, a single condensate into a fragmented condensate many-body state. Although MCTDHB provides an important tool to describe the many-body physics of interacting bosons, the method therefore lacks the possibility to directly connect the phenomena of condensation and

fragmentation.

Here, critically examining Dirac-Frenkel's principle and the TDVP, and adopting alternatively McLachlan's principle for truncated many-body evolution, we improve on the previous multi-configurational Hartree methods, and solve the singularity problem of a noninvertible SPDM. In the process, we will also validate the resulting equations of MCTDHB in a different manner, however additionally offering a straightforward handling of the exceptional evolution points related to the singularity of the SPDM.

2. Variational Principles

Let us now discuss the possible variational principles in more detail. We are aiming at finding an approximate solution of the many-body Schrödinger equation when the state $|\Phi\rangle$ is restricted. McLachlan's principle [7], which was presented in 1963 as a new version of Frenkel's principle, requires the minimization of the error or remainder of this approximate solution from the exact evolution. The time evolution of any state is dictated by Schrödinger's equation, $i\partial_t|\Phi\rangle = \hat{H}|\Phi\rangle$. In other words, the evolution of state is determined by the Hamiltonian at any moment. But to make the state $|\Phi\rangle$ manipulable, we are generally forced to restrict or confine the state $|\Phi\rangle$ into some simple and computationally feasible forms. With the state $|\Phi\rangle$ in restricted form, $[i\partial_t - \hat{H}]|\Phi\rangle$ cannot be exactly zero in general. Therefore, McLachlan's principle aims at finding the approximate solution which minimizes the positive semidefinite error measure $\langle\Phi|[i\partial_t - \hat{H}]^\dagger[i\partial_t - \hat{H}]|\Phi\rangle$. The details of the corresponding procedure will be rephrased in section 2.2, after introducing a concrete way to restrict the many-body state in a computationally feasible form.

Hence it is guaranteed that the equation of motion obtained from McLachlan's principle follows the exact evolution most similarily under given constraints. The most appealing feature of McLachlan's principle is thus that it is a quite intuitive principle. Since it offers the possibility to evaluate the error directly, we can intermediately, monitoring the error, increase the number of orbitals in the truncated field operator expansion, i.e. truncate the state less, to assure accuracy of the result. Alternatively, to save computational costs and time, the number of orbitals can also be decreased intermediately, i.e. by truncating the state more, in particular in cases where decreasing the number of orbitals does not affect the accuracy of result significantly. Our scheme, described in detail below, in which McLachlan's principle is applied, therefore offers the opportunity to dynamically adjust the truncation of field operators or the state itself properly during computational time evolution, since we can monitor the error. As a particular benefit, a convergence test, mandatory for MCTDHB, is unneccessary, as we can directly obtain an error which indicates automatically how well our approach describes the interacting system of bosons.

On the other hand, the TDVP which was carried out in MCTDHB [9] requires stationarity of action $\delta S = 0$. This does not necessarily mean an extremum (minimum or maximum) of the action. Though stationary points include local extrema, the principle practically imposes only stationarity of the action: The equation of motion comes from stationary point of the action, which is not even necessarily a local minimum or maximum.

In many-body quantum mechanics, the action is written in terms of an expectation value of an operator-valued functional:

$$\begin{aligned} S = &\int \mathrm{d}t \int \mathrm{d}\vec{x}\, \big\langle \Phi \big| \left[\frac{1}{2m} \sum_{i=1}^{3} \big(\partial_i \hat{\Psi}^\dagger(\vec{x})\big)\big(\partial_i \hat{\Psi}(\vec{x})\big) + V_{\mathrm{trap}}(\vec{x},t)\hat{\Psi}^\dagger(\vec{x})\hat{\Psi}(\vec{x}) \right] \big| \Phi \big\rangle \\ &+ \frac{1}{2} \int \mathrm{d}t \iint \mathrm{d}\vec{x}_\alpha \mathrm{d}\vec{x}_\beta\, \big\langle \Phi \big| V(\vec{x}_\alpha, \vec{x}_\beta) \hat{\Psi}^\dagger(\vec{x}_\alpha)\hat{\Psi}^\dagger(\vec{x}_\beta)\hat{\Psi}(\vec{x}_\beta)\hat{\Psi}(\vec{x}_\alpha) \big| \Phi \big\rangle \\ &- \int \mathrm{d}t\, \big\langle \Phi \big| \left[\frac{\big[i\partial_t\big] + \big[i\partial_t\big]^\dagger}{2} \right] \big| \Phi \big\rangle \end{aligned} \tag{1}$$

which is in quantum mechanical correspondence to the classical Lagrangian action. Here, $V_{\mathrm{trap}}(\vec{x},t)$ is the (in general time-dependent) scalar trap potential confining the atoms, $V(\vec{x}_\alpha, \vec{x}_\beta)$ is the two-body interaction potential, and m the mass of bosons. This is a real-valued functional of the many-body state $|\Phi\rangle$ [15]. Sometimes the action is simply expressed as $S = \int \mathrm{d}t\, \langle \Phi | \hat{H} - i\partial_t | \Phi \rangle$. Variationally changing the state $|\Phi\rangle$ and the temporal change of the state $\partial_t|\Phi\rangle$, we find the evolution of the state around the stationary action point.

But here a problem occurs. When the form of the state is restricted or truncated for computational reasons in the sense that the state resides in a sub-Hilbert space, it is questionable whether the equation of motion obtained in the sub-Hilbert space leads to an evolution most similarily to the exact one obtained with the unlimited full Hilbert space. Even though the equation of motion obtained variationally with a non-truncated state can give the correct many-body Schrödinger equation, we cannot rely on the correctness of the equation in case the state is truncated. The path of stationary action with limitations imposed on the path can in principle deviate far from the one obtained without any constraints on the path.

As a simple example, when we restrict the state to have only an overall phase change, i.e. $|\Phi(t)\rangle = e^{-i\Omega t}|\Phi\rangle$, the action becomes $S = \int \mathrm{d}t \big(\langle \hat{H} \rangle - \Omega \big)$. Depending on the value of Ω, the action can be positive or negative. Actually there is no upper bound and lower bound on this action. Even worse, for some types of constrained states, there can be no stationary point of the action at all. So when applying the TDVP, at least the convergence upon increasing the number of orbitals, i.e., loosening the constraints, must be tested for every specific problem, to ensure the validity of the results. This is because, in contrast with McLachlan's principle, there is no direct error indicator in the TDVP which controls the accuracy of the approximation.

The earliest variational principle for the approximate solution of many-body dynamics is Dirac-Frenkel's principle [5, 6], which requires

$$\langle \delta\Phi | \hat{H} - i\partial_t | \Phi \rangle = 0, \tag{2}$$

where $\delta\Phi$ denotes possible variations of the many-body state Φ with respect to the variational parameters. The equation is quite similar to the TDVP when the action is given by $S = \int \mathrm{d}t \langle \Phi | \hat{H} - i\partial_t | \Phi \rangle$. The difference and (possible) equivalences between Dirac-Frenkel's, McLachlan's and other variational principles have been extensively discussed in the past [8, 14]. In [8], it is concluded that if the relevant manifold, i. e. the sub-Hilbert space, can be parametrized by

pairs of complementary parameters, the above mentioned principles are equivalent. In [14], it is insisted that both Dirac-Frenkel's and McLachlan's variational principles are equivalent if both $\delta\Phi$ and $\delta\Phi^*$ are possible independent variations. But the "equivalence" merely implies the same resulting equation under some given conditions, not the equivalence of the principles themselves. In addition, it appears doubtful that $\delta\Phi$ and $\delta\Phi^*$ are possible independent variations since $\delta\Phi^*$ is simply the complex conjugate of $\delta\Phi$. Furthermore, as explained in detail later, principles which result in the problem of a noninvertible SPDM, which was alluded to already in the above, lack some information in comparison to McLachlan's principle, which resolves this problem.

In summary, comparing the three variational principles, McLachlan's principle appears to be most suitable for finding a truncated many-body dynamics which approximates the real dynamics of interacting bosons. Adopting McLachlan's principle, the variationally optimal truncation of the many-body dynamics of interactiong bosons can be adaptively controlled with a monitored error.

2.1. Truncating a many-body state

The limited or restricted forms of the state $|\Phi\rangle$ for the truncated many-body dynamics can in principle take any form. In the simplest case, assuming that the occupation numbers of bosons concentrate in one orbital for the whole time of evolution, we can treat the many-body state with one single-particle orbital. More generally, the state will reside in a sub-Hilbert space of a specific form. An easily extendible and flexible form of the limitation on the size of the Hilbert space is the multiconfigurational time-dependent Hartree wavefunction ansatz, in which the many-body state of bosons is described as a linear combination of permanents $|\vec{n}\rangle$, with a finite number M of orthonormalized time-dependent single-particle orbitals. Increasing the number M of orbitals, we can easily extend the time-dependent sub-Hilbert space $\mathcal{M}(t)$. The basic steps to be followed in the procedure are as follows.

Firstly, the many-body Hamiltonian is given by

$$\begin{aligned}\hat{H} = &\int \mathrm{d}\vec{x}\ \ \hat{\Psi}^\dagger(\vec{x})\bigg[-\frac{\nabla^2}{2m}+V_{\mathrm{trap}}(\vec{x})\bigg]\hat{\Psi}(\vec{x})\\ &+\frac{1}{2}\iint \mathrm{d}\vec{x}_\alpha \mathrm{d}\vec{x}_\beta\, \hat{\Psi}^\dagger(\vec{x}_\alpha)\hat{\Psi}^\dagger(\vec{x}_\beta)V(\vec{x}_\alpha,\vec{x}_\beta)\hat{\Psi}(\vec{x}_\beta)\hat{\Psi}(\vec{x}_\alpha).\end{aligned} \tag{3}$$

With a complete set of basis orbitals, the field operators of creation and annihilation of particles are expressed by the expansions

$$\hat{\Psi}^\dagger(\vec{x}) = \sum_{i=1}^{\infty}\hat{a}_i^\dagger\phi_i^*(\vec{x}) \qquad \text{and} \qquad \hat{\Psi}(\vec{x},t) = \sum_{i=1}^{\infty}\hat{a}_i\phi_i(\vec{x},t). \tag{4}$$

Using these, the Hamiltonian can be written

$$\hat{H} = \sum_{i,j=1}^{\infty}\epsilon_{ij}\hat{a}_i^\dagger\hat{a}_j + \frac{1}{2}\sum_{i,j,k,l=1}^{\infty}V_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l \tag{5}$$

where the single-particle matrix elements are

$$\epsilon_{ij} = \int \mathrm{d}\vec{x}\ \ \phi_i^*(\vec{x})\bigg[-\frac{\nabla^2}{2m}+V_{\mathrm{trap}}(\vec{x})\bigg]\phi_j(\vec{x}), \tag{6}$$

while the two-body interaction is represented by

$$V_{ijkl} = \iint \mathrm{d}\vec{x}_1 \mathrm{d}\vec{x}_2 \; \phi_i^*(\vec{x}_\alpha)\phi_j^*(\vec{x}_\beta)V(\vec{x}_\alpha,\vec{x}_\beta)\phi_k(\vec{x}_\beta)\phi_l(\vec{x}_\alpha). \tag{7}$$

We abbreviate sometimes, for the sake of convenience,

$$\hat{a}_{ij}^\dagger \equiv \hat{a}_i^\dagger \hat{a}_j, \quad \hat{a}_{ijkl}^{\dagger\dagger} \equiv \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l, \quad \hat{a}_{ijk}^{\dagger\dagger} \equiv \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k, \quad \hat{a}_{ijk}^\dagger \equiv \hat{a}_i^\dagger \hat{a}_j \hat{a}_k \tag{8}$$

and so on. Then, the Hamiltonian can be written in short-hand form as $\hat{H} = \hat{h} + \frac{1}{2}\hat{V} = \sum_{i,j=1}^{\infty} \epsilon_{ij}\hat{a}_{ij}^\dagger + \frac{1}{2}\sum_{i,j,k,l=1}^{\infty} V_{ijkl}\hat{a}_{ijkl}^{\dagger\dagger}$.

To find the many-body ground state $|G\rangle$, we have to minimize the energy expectation value $E_G = \langle G|\hat{H}|G\rangle$. Without any restrictions on the state $|G\rangle$, the actual exact ground state will be found. However realistically, we cannot describe a state exactly as this will in general require infinitely many orbitals. So we confine the state into a space of finite dimension, i.e. using only finite number M of orbitals, which is computationally feasible,

$$|G^{\mathcal{M}}\rangle = \sum_{\vec{n}\in\mathcal{M}} C_{\vec{n}}|\vec{n}\rangle. \tag{9}$$

The above is regarded as the truncation of the many-body bosonic state. Here $|\vec{n} \in \mathcal{M}\rangle$ indicates a normalized Fock state or a permanent

$$|\vec{n}\rangle \equiv \frac{\left(\hat{a}_1^\dagger\right)^{n_1}\left(\hat{a}_2^\dagger\right)^{n_2}\cdots\left(\hat{a}_M^\dagger\right)^{n_M}}{\sqrt{n_1!n_2!\cdots n_M!}}|\mathrm{vac}\rangle \quad \text{with} \quad \sum_{i=1}^{M} n_i = N, \tag{10}$$

which is a N particle state of which the individual members are composed of n_1 particles in $\phi_1(\vec{x})$ orbital, n_2 particles in $\phi_2(\vec{x})$ orbital, $\cdots$, and n_M particles in $\phi_M(\vec{x})$ orbital. These M orbitals must be orthonormalized to each other.

$$\int \mathrm{d}\vec{x} \; \phi_i^*(\vec{x})\phi_j(\vec{x}) = \delta_{ij}. \tag{11}$$

These orbitals compose the sub-Hilbert manifold spanned by M orthonormal orbitals, which will be denoted by $\mathcal{M}$ in our context. The operators of creation and annihilation on these are related to the field operators in position space by the inversion of (4),

$$\hat{a}_i = \int \mathrm{d}\vec{x} \; \hat{\Psi}(\vec{x})\phi_i^*(\vec{x}) \qquad \text{and} \qquad \hat{a}_i^\dagger = \int \mathrm{d}\vec{x} \; \hat{\Psi}^\dagger(\vec{x})\phi_i(\vec{x}). \tag{12}$$

Here, a sub-Hilbert space spanned by $\sum_{i=1}^{M} c_i\phi_i(\vec{x})$ is to be chosen so as to describe the ground state optimally. And the coefficients $C_{\vec{n}}$ which give minimum of energy are to be determined, too. Then, $|G^{\mathcal{M}}\rangle$ can be considered as optimal truncation of the actual ground state $|G\rangle$. The details on how to proceed concretely will follow below in section 4.

In the time-evolving case, we change not only the coefficients $C_{\vec{n}}$ along time, but also the sub-Hilbert space $\mathcal{M}$ changes with time. With a time-varying truncation of the many-body state, we can express the state as

$$|\Phi(t)\rangle = \sum_{\vec{n}\in\mathcal{M}(t)} C_{\vec{n}}(t)|\vec{n};t\rangle, \tag{13}$$

with time-varying orbitals and their conjugate creation operators

$$\hat{a}_i^\dagger(t) = \int \mathrm{d}\vec{x}\ \hat{\Psi}^\dagger(\vec{x})\phi_i(\vec{x},t). \tag{14}$$

This approach was also incorporated in MCTDHB [9]. The time differentiation of the state $|\Phi(t)\rangle$ then becomes

$$i\partial_t|\Phi(t)\rangle = \sum_{\vec{n}\in\mathcal{M}(t)} \Big[\big(i\partial_t C_{\vec{n}}(t)\big)|\vec{n};t\rangle + C_{\vec{n}}(t)\sum_{i=1}^{M}\int \mathrm{d}\vec{x}\ \big(i\partial_t\phi_i(\vec{x},t)\big)\hat{\Psi}^\dagger(\vec{x})\hat{a}_i|\vec{n};t\rangle\Big]. \tag{15}$$

Expanding $\partial_t\phi_i(\vec{x},t)$ with a complete basis yields

$$i\partial_t\phi_i(\vec{x},t) = \sum_{k=1}^{\infty} t_{ki}(t)\phi_k(\vec{x},t). \tag{16}$$

where the matrix t_{ki} for $1 \le k \le M$ indicates an *inner rotation* inside the sub-Hilbert space, whereas t_{ki} for $k > M$ changes sub-Hilbert space itself. Integrating both sides after multiplying with $\phi_k^*(\vec{x},t)$, we obtain

$$t_{ki}(t) = \int \mathrm{d}\vec{x}\ \phi_k^*(\vec{x},t)\big(i\partial_t\phi_i(\vec{x},t)\big). \tag{17}$$

Then Eq. (15) can be expressed in the alternative form

$$i\partial_t|\Phi(t)\rangle = \sum_{\vec{n}\in\mathcal{M}(t)} \Big[\big(i\partial_t C_{\vec{n}}(t)\big)|\vec{n};t\rangle + C_{\vec{n}}(t)\sum_{k=1}^{\infty}\sum_{i=1}^{M} t_{ki}\hat{a}_{ki}^\dagger|\vec{n};t\rangle\Big]. \tag{18}$$

These preliminaries will be used in the following sections, by providing the tools for describing the truncated state $|\Phi\rangle$ optimally.

2.2. Adapting the number of orbitals

The governing equation of MCTDHB which comes from either Dirac-Frenkel's principle or TDVP implies that the SPDM must be always invertible, not only initially but also at any instant afterwards. We quote here the equation (26) in [9], which is

$$i\partial_t\phi_k(\vec{x},t) = \sum_{l=M+1}^{\infty}\Big[\epsilon_{lk} + \sum_{i,n,p,q=1}^{M}\langle\rho\rangle_{ki}^{-1}\langle\hat{a}_{inpq}^{\dagger\dagger}\rangle V_{lnpq}\Big]\phi_l(\vec{x},t) \tag{19}$$

in our notation, where $\langle\rho\rangle_{ki}^{-1}$ represents the inverse of the SPDM $\langle\rho_{ij}\rangle \equiv \langle\hat{a}_{ij}^\dagger\rangle$. In [9], it seems to be taken for granted that the SPDM is always invertible. When the SPDM becomes noninvertible, however, the MCTDHB method in fact suddenly fails. For example, when the whole bosons of our interest resides initially in single orbital, MCTDHB cannot propagate this pure condensate into any fragmented state. As a consequence, the method does not provide a way to find the form of the second orbital.

To decrease the sub-Hilbert space or the number of orbitals is not an issue. We can simply eliminate those orbitals with an occupation number not of order

N. However, to increase the sub-Hilbert space dimension, that is the number of orbitals M, becomes difficult since an increase of the sub-Hilbert space and an additional orbital must be set up optimally. Noninvertibility of the SPDM can obviously also happen dynamically. Unoccupied orbitals or scarcely occupied orbitals thus cause a problem with the dynamics of MCTDHB. These problems cannot be resolved by Dirac-Frenkel's principle or the TDVP. As McLachlan's principle is based on requiring that the least error is acquired during time evolution, we may resolve this problem by finding an additional orbital which minimizes the error, as will be expounded in detail below.

McLachlan's principle does not use the action, but the concept of error or remainder. We know the exact form of the many-body Schrödinger equation. It is $i\partial_t|\Phi\rangle = \hat{H}|\Phi\rangle$ with the full Hamiltonian Eq. (3) in second quantization form. Since the exact calculation is too cumbersome, we can represent the state by the relatively simple multiconfigurational time-dependent Hartree form. The remainder from exact evolution in any case becomes

$$\big[i\partial_t - \hat{H}\big]\big|\Phi\big\rangle. \tag{20}$$

In this expression, the left part $i\partial_t|\Phi\big\rangle$ is an evolution of the state $|\Phi\rangle$ in its limited, truncated form and the right part $\hat{H}|\Phi\big\rangle$ represents the exact evolution. Here, the initial state, for either part, is specified in its truncated form, while the Hamiltonian $\hat{H}$ is not truncated.

A quantitative measure of the instantaneous error is then

$$\big\langle\Phi\big|\big[i\partial_t - \hat{H}\big]^\dagger\big[i\partial_t - \hat{H}\big]\big|\Phi\big\rangle \geq 0, \tag{21}$$

which is (by definition) positive semidefinite. We have to minimize this error by varying the truncated state in Eq. (13).

3. Method of steepest constrained descent

In this section, we describe the basic method which will be used to find both a minimum of energy and a minimum of instantaneous error in the following sections. Since we use complex variables and complex functions, the well-known method of Lagrange multipliers will here be carefully extended to one with complex numbers. In addition, we introduce the method of steepest *constrained* descent, which propagates an initial trial estimate (the many-body state) by steepest descent under the given constraints toward an approximate minimum point. The method provides a simplified way to find the latter, and is introduced because a fully self-consistent solution is frequently forbiddingly difficult to find from the equations following from using the bare method of Lagrange multipliers.

3.1. Method of Lagrange multipliers with complex numbers

In mathematical optimization, i.e. when we want to find a minimum or maximum of a continuous differentiable function $f(\vec{x})$ subject to some constraints $g_l(\vec{x}) = \text{const}$, where the index l enumerates the constraints, the method of Lagrange multipliers is widely used. Providing conditions for stationary points subject under the constraints, it provides a strategy for finding minima and

maxima. Comparing the obtained values at the stationary points obtained, we can determine which point is a minimum or maximum.

With complex variables or complex functions, some caution is however necessary. As one complex variable z_k corresponds to two real variables $a_k + ib_k$, both real and imaginary parts of z_k should satisfy the Lagrange formula,

$$\frac{\partial f}{\partial a_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial a_k} = 0 \qquad \text{and} \qquad \frac{\partial f}{\partial b_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial b_k} = 0, \tag{22}$$

where f and g_l are given real-valued functions. There is a compact way to express the two real equations above.

$$\begin{aligned} &\frac{\partial f}{\partial z_k^*} - \sum_l \lambda_l \frac{\partial g_l}{\partial z_k^*} \\ &= \frac{1}{2}\frac{\partial f}{\partial a_k} - \frac{1}{2i}\frac{\partial f}{\partial b_k} - \sum_l \lambda_l \left(\frac{1}{2}\frac{\partial g_l}{\partial a_k} - \frac{1}{2i}\frac{\partial g_l}{\partial b_k} \right) \\ &= \frac{1}{2}\left(\frac{\partial f}{\partial a_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial a_k} \right) - \frac{1}{2i}\left(\frac{\partial f}{\partial b_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial b_k} \right) = 0. \end{aligned} \tag{23}$$

Since the functions f and g_l's are real-valued, the derivatives with respect to real variable a_k's and b_k's are also real-valued functions. Hence the above complex equation requires that both real and imaginary parts would be zero independently. This is not because z_k and z_k^* are possible independent variables. z_k and its conjugate z_k^* are definitely dependent variables. We use this just as a compact way of expression for two real equations, using partial derivatives with respect to the complex variable. Here, we need to be very cautious using the partial derivatives. When a function f is given with several variables, the partial derivative $\partial f/\partial z$ means a differentiation with respect to only that variable z even though others such as z^*, a, b are dependent on z. We should also be careful with which variables the function is expressed. Commonly $\partial f/\partial z$ means $\partial f(z, z^*)/\partial z$ and $\partial f/\partial a$ means $\partial f(a, b)/\partial a$. Only when there is no possible source of confusion, we drop these explicit indications for the sake of convenience.

The formulas change if the constraints g_l are given in complex form. A single complex constraint corresponds to two real constraints,

$$g_l = g_l^{(R)} + i g_l^{(I)} = \text{const.} \tag{24}$$

Then, with two groups of real Lagrange multipliers for the real part and imaginary parts of the complex constraints,

$$\begin{aligned} \frac{\partial f}{\partial x_k} &= \sum_l \left[\lambda_l^{(R)} \frac{\partial g_l^{(R)}}{\partial x_k} + \lambda_l^{(I)} \frac{\partial g_l^{(I)}}{\partial x_k} \right] \\ &= \sum_l \left[\frac{\lambda_l^{(R)}}{2} \Big[\frac{\partial g_l}{\partial x_k} + \frac{\partial g_l^*}{\partial x_k} \Big] + \frac{\lambda_l^{(I)}}{2i} \Big[\frac{\partial g_l}{\partial x_k} - \frac{\partial g_l^*}{\partial x_k} \Big] \right] \\ &= \sum_l \left[\Big[\frac{\lambda_l^{(R)}}{2} + \frac{\lambda_l^{(I)}}{2i} \Big] \frac{\partial g_l}{\partial x_k} + \Big[\frac{\lambda_l^{(R)}}{2} - \frac{\lambda_l^{(I)}}{2i} \Big] \frac{\partial g_l^*}{\partial x_k} \right]. \end{aligned} \tag{25}$$

Introducing a complex Lagrange multiplier $\lambda_l = \frac{1}{2}[\lambda_l^{(R)} - i\lambda_l^{(R)}]$,

$$\frac{\partial f}{\partial x_k} = \sum_l \left[\lambda_l \frac{\partial g_l}{\partial x_k} + \lambda_l^* \frac{\partial g_l^*}{\partial x_k}\right]. \tag{26}$$

Complex constraints come with complex Lagrange multipliers. Then, the complex conjugate form of the constraints must be added. When both variables and constraints are in complex form, the equations will be represented by

$$\frac{\partial f}{\partial z_k^*} = \sum_l \left[\lambda_l \frac{\partial g_l}{\partial z_k^*} + \lambda_l^* \frac{\partial g_l^*}{\partial z_k^*}\right] \tag{27}$$

or equivalently

$$\frac{\partial f}{\partial z_k} = \sum_l \left[\lambda_l \frac{\partial g_l}{\partial z_k} + \lambda_l^* \frac{\partial g_l^*}{\partial z_k}\right]. \tag{28}$$

Case by case, we can choose the simpler form of the two equivalent complex equations (27) and (28) above.

3.2. Approaching along steepest constrained descent

Even when we have found the equations for extreme or stationary points, we usually cannot find those points directly from the equations except for some simple cases. What we conventionally can do at most is, in general, to give some approximate estimates of an extremal point. These estimates would not satisfy the stationarity condition exactly. Therefore, to find the actual accurate point of extremum which fulfills the stationarity condition found by the method of Lagrange multipliers, we have to propagate the initial trial point of departure, which is in a truncated many-body state space in our context, to the actual minimum or maximum point.

Allocating a pseudo time τ along the path on which the point in the configuration space (the many-body state in our context) moves, we can consider the rate of change

$$\frac{df}{d\tau} = \sum_k \frac{\partial f}{\partial x_k}\frac{dx_k}{d\tau}, \tag{29}$$

with respect to the pseudo time τ. The rate of change $\frac{df}{d\tau}$ indicates how rapidly the value of f changes at $\vec{x}(\tau)$ along the path toward $\frac{d\vec{x}}{d\tau}$. The Lagrange formula Eq. (22) comes from the condition that $\frac{df}{d\tau} = 0$ for any variation of the x_k, i.e. any $\frac{dx_k}{d\tau}$, under given constraints. In non-stationary points, the path which gives the smallest (biggest) value of $\frac{df}{d\tau}$ will be called the steepest descent (ascent). However, without any limit on the velocity of the variable changes $\frac{d\vec{x}}{d\tau}$, the rate of change $\frac{df}{d\tau}$ would be also unlimited. In addition, any given points along the path must still satisfy the constraints $g_l(\vec{x}(\tau)) = \text{const}$, as we are trying to find the minimum or maximum of $f(\vec{x})$ under the given constraints. So minimizing (maximizing) the rate of change $df/d\tau$ Eq. (29) within the constrained path, i.e.

$$\frac{dg_l}{d\tau} = \sum_k \frac{\partial g_l}{\partial x_k}\frac{dx_k}{d\tau} = 0 \tag{30}$$

and under a closed topology which can be, for example, taken to be a hypersphere

$$\sum_k \left(\frac{dx_k}{d\tau}\right)^2 = \text{const}, \tag{31}$$

we can propagate the point along the steepest *constrained* descent (ascent). Here, what we are varying is the speed of variable change, i.e. the set $\{\frac{dx_k}{d\tau}\}$. The closed topology which we have chosen limits the overall rate of change (speed), of the variables $|\frac{d\vec{x}}{d\tau}|$, so that the rate of change $\frac{df}{d\tau}$ does not diverge. Without a closed topology which limits the change of variables, we would not be able in general to find the steepest path since it possibly diverges with the variable changes under an open topology. To be specific, in our context, the function f to be minimized corresponds to the energy expectation value $E_{G^{\mathcal{M}}}$ (or the instantaneous error $\langle[i\partial_t - \hat{H}]^\dagger[i\partial_t - \hat{H}]\rangle$), the constraints g_l to $\sum_{\vec{n}} C^*_{\vec{n}} C_{\vec{n}} = 1$ and $\int \mathrm{d}\vec{x}\ \phi^*_i(\vec{x})\phi_j(\vec{x}) = \delta_{ij}$ for $i, j \leq M$ (or time derivatives of them); therefore l goes from 1 to $(1 + M^2)$, and the variables x_k correspond to the coefficients $C_{\vec{n}}$ and the orbitals $\phi_k(\vec{x})$ (respectively their time derivatives).

As we minimize (maximize) the rate of change $df/d\tau$ Eq. (29) under the closed topology with respect to the rate of change, $\frac{dx_k}{d\tau}$, we use again the method of Lagrange multipliers which gives the condition of the stationary $\frac{df}{d\tau}$ in the form

$$\frac{\partial f}{\partial x_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial x_k} - 2\lambda \frac{dx_k}{d\tau} = 0, \tag{32}$$

for all possible k. The simple linearity of Eq. (29, 30) on $\frac{dx_k}{d\tau}$ provides directly the result

$$\frac{dx_k}{d\tau} = \mp\Delta(\tau)\left[\frac{\partial f}{\partial x_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial x_k}\right] \tag{33}$$

from Eq. (32). Here we transformed the multiplier λ into a new convenient expression $\mp\Delta(\tau) \equiv \frac{1}{2\lambda(\tau)}$. The undetermined Lagrange multipliers $\lambda_l(\tau)$ and $\Delta(\tau)$ are then determined by the constraints Eq. (30) and Eq. (31). Inserting Eq. (33) into Eq. (30),

$$\begin{aligned} &\mp \Delta(\tau) \sum_k \frac{\partial g_m}{\partial x_k}\left[\frac{\partial f}{\partial x_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial x_k}\right] = 0 \\ \Rightarrow \quad &\sum_k \frac{\partial f}{\partial x_k}\frac{\partial g_m}{\partial x_k} = \sum_l \lambda_l \sum_k \frac{\partial g_l}{\partial x_k}\frac{\partial g_m}{\partial x_k}. \end{aligned} \tag{34}$$

Introducing the inverse A^{-1}_{mn} of the symmetric matrix $A_{lm} \equiv \sum_k \frac{\partial g_l}{\partial x_k}\frac{\partial g_m}{\partial x_k}$, λ_l is determined to be

$$\lambda_l = \sum_{k,m} \frac{\partial f}{\partial x_k}\frac{\partial g_m}{\partial x_k} A^{-1}_{ml}. \tag{35}$$

Though $\Delta(\tau)$ is also to be determined to satisfy Eq. (31), the 'const' on the right side of Eq. (31) is just a constant whose value is unimportant. Unless we fix the size of the topological constraint 'const', $\Delta(\tau)$ can be whatever function of τ. But since the rate of change $\frac{df}{d\tau}$ should be negative (positive) to approach a minimum (maximum) of $f(\vec{x})$, we choose $\Delta(\tau)$ to be always positive definite, i.e. $\Delta(\tau) > 0$ for all τ. Furthermore, we take a minus (plus) in front of the right-hand side of Eq. (33) to approach a minimum (maximum) of $f(\vec{x})$.

The point in configuration space will eventually arrive on a neighboring local minimum or maximum along the path

$$\vec{x}(\tau = T) = \vec{x}(\tau = 0) + \int_0^T \mathrm{d}\tau \, \frac{d\vec{x}}{d\tau}(\tau), \tag{36}$$

where $x_k(\tau = 0)$ is the initially estimated point and $\frac{d\vec{x}}{d\tau}(\tau)$ represents the direction of the steepest constrained descent (ascent) under a given topology. The path will strongly depend on the choice of topology. To save calculational time, we can fix some variables alternatively. In other words, setting $dx_l/d\tau = 0$ for some set $\{l\}$ within some pseudo-time τ span, we change only the other variables along the steepest constrained descent. Then the hypersphere topological constraint Eq. (31) on the velocity of the variable, $\frac{d\vec{x}}{d\tau}$, changes into

$$\frac{dx_{l\text{'s}}}{d\tau} = 0 \quad \text{and} \quad \sum_{k \neq \{l\}} \left(\frac{dx_k}{d\tau}\right)^2 = \text{const.} \tag{37}$$

It approaches in any case a point which has less (more) numerical value of $f(\{x_k\})$ than the current point, following a stepwise path. As a simple example, when $f(a, b)$ is a function of two variables, we can change a and b separately to approach a neighboring minimum. When $\frac{\partial f}{\partial a} > 0$, we decrease a until $\frac{\partial f}{\partial a} = 0$. After then, testing $\frac{\partial f}{\partial b}$ at that point, we propagate b until $\frac{\partial f}{\partial b} = 0$. Successively and iteratively we change a and b until both $\frac{\partial f}{\partial a} = 0$ and $\frac{\partial f}{\partial b} = 0$ are met. Along this stepwise path, the point propagates to the neighboring minimum. By this means, which is a separation of the change of variables, we can obtain an efficient and thus fast procedure for a concrete computation.

As the steepest descent (ascent) does not gurantee the shortest path to the minimum (maximum), a flexible and adaptive choice of topology is crucial to save time and effort. However, the hypersphere topology and separation of the change of variables will be sufficient in most practical cases.

In summary, the method of steepest constrained descent (ascent) guarantees that the configuration space point approaches a neighboring local minimum (maximum) of $f(\vec{x})$, by propagating the point toward

$$\frac{dx_k}{d\tau} = \mp\Delta(\tau)\left[\frac{\partial f}{\partial x_k} - \sum_l \lambda_l \frac{\partial g_l}{\partial x_k}\right] \tag{38}$$

for hypersphere topology. Here $\lambda_l(\tau)$ is given by Eq. (35) at each point, and $\Delta(\tau)$ is any arbitrary positive function of τ, which would be chosen in any convenient way during the actual computation. To approach a minimum (maximum) of $f(\vec{x})$, we take minus (plus) in front of the right hand side of Eq. (38).

With complex variables and complex constraints, using Eq. (27), this will be simplified as

$$\frac{dz_k}{d\tau} = \frac{da_k}{d\tau} + i\frac{db_k}{d\tau} = \mp\Delta(\tau)\left[\frac{\partial f}{\partial z_k^*} - \sum_l \left[\lambda_l \frac{\partial g_l}{\partial z_k^*} + \lambda_l^* \frac{\partial g_l^*}{\partial z_k^*}\right]\right]. \tag{39}$$

We have ignored that $\Delta(\tau)$ should be doubled on the right-hand side since $\Delta(\tau)$ can be arbitrarily chosen, i.e. we put $2\Delta(\tau) \to \Delta(\tau)$.

4. Minimizing the energy of the truncated many-body state

4.1. Variational method with Lagrange multipliers

Before investigating the dynamics, let us demonstrate the time-independent scheme first. To find the many-body ground state, we have to minimize the energy expectation value

$$E_{G^{\mathcal{M}}} = \langle G^{\mathcal{M}}|\hat{H}|G^{\mathcal{M}}\rangle = \Big[\sum_{\vec{m}\in\mathcal{M}}\langle\vec{m}|C^*_{\vec{m}}\Big]\hat{H}\Big[\sum_{\vec{n}\in\mathcal{M}}C_{\vec{n}}|\vec{n}\rangle\Big] \tag{40}$$

by varying the coefficients $C_{\vec{n}}$'s and the set of M orbitals $\{\phi_i\}$, subject to the $(1+M^2)$ constraints

$$\sum_{\vec{n}} C^*_{\vec{n}}C_{\vec{n}} = 1 \qquad (1 \text{ constraint}) \tag{41}$$

and

$$\int \mathrm{d}\vec{x}\ \phi^*_i(\vec{x})\phi_j(\vec{x}) = \delta_{ij} \quad \text{for } i,j \le M \qquad (M^2 \text{ constraints}). \tag{42}$$

The variation with respect to the expansion coefficients $C_{\vec{n}}$ gives

$$\frac{\partial E_{G^{\mathcal{M}}}}{\partial C^*_{\vec{n}}} = \langle\vec{n}|\hat{H}\sum_{\vec{m}in\mathcal{M}}C_{\vec{m}}|\vec{m}\rangle = \lambda C_{\vec{n}} = E_{G^{\mathcal{M}}}C_{\vec{n}}, \tag{43}$$

where $\vec{n}\in M$. We have a real functional E_{G^M} Eq. (40) to be minimized, and one real equation of constraint Eq. (41), with $\frac{(N+M-1)!}{N!(M-1)!}$ complex variables $C_{\vec{n}}$ when we fix the total number of bosons N. The undetermined Lagrange multiplier λ which has to be real is determined to be $E_{G^{\mathcal{M}}}$ with the help of constraint Eq. (41).

Using the properties $\epsilon^*_{ij} = \epsilon_{ji}$, $V_{ijkl} = V_{jilk}$ and $V^*_{ijkl} = V_{lkji} = V_{klij}$, we can express the above equation explicitly as

$$\begin{aligned}
&\langle\vec{n}|\hat{H}\sum_{\vec{m}\in\mathcal{M}}C_{\vec{m}}|\vec{m}\rangle = E_{G^{\mathcal{M}}}C_{\vec{n}} \\
&= \sum_l\Big[\epsilon_{ll} + \frac{1}{2}V_{llll}(n_l-1) + \frac{1}{2}{\sum_k}'(V_{lklk}+V_{lkkl})n_k\Big]n_lC_{\vec{n}} \\
&+ {\sum_{j,l}}'\Big[\epsilon_{lj} + V_{lllj}(n_l-1) + V_{ljjj}n_j + {\sum_k}'(V_{lkkj}+V_{lkjk})n_k\Big]\sqrt{(n_j+1)n_l}C_{\vec{n}^j_l} \\
&+ \frac{1}{2}{\sum_{j,l}}'V_{lljj}\sqrt{(n_j+2)(n_j+1)(n_l-1)n_l}C_{\vec{n}^{jj}_{ll}} \\
&+ \frac{1}{2}{\sum_{i,j,l}}'V_{llji}\sqrt{(n_i+1)(n_j+1)(n_l-1)n_l}C_{\vec{n}^{ij}_{ll}} \\
&+ \frac{1}{2}{\sum_{j,k,l}}'V_{lkjj}\sqrt{(n_j+2)(n_j+1)n_kn_l}C_{\vec{n}^{jj}_{kl}} \\
&+ \frac{1}{2}{\sum_{i,j,k,l}}'V_{lkji}\sqrt{(n_i+1)(n_j+1)n_kn_l}C_{\vec{n}^{ij}_{kl}},
\end{aligned} \tag{44}$$

where the primed summation $\sum'$ is performed such that different indices can have only different values. For example, summations over two and three indices are $\sum_{j,l}{}' \equiv \sum_j \sum_{l\neq j}$, $\sum_{i,j,l}{}' \equiv \sum_i \sum_{j\neq i} \sum_{l\neq i \text{ or } j}$, and $\sum_k{}'$ inside a bracket means $\sum_{k\neq(\text{the other indices})}$. Though Eq. (44) is just an eigenvalue equation with fixed matrix components, the terms ϵ_{ij} and V_{ijkl} are matrix elements depending on the orbitals, which are to be determined as follows.

For variation with respect to the orbitals $\{\phi_k\}$, functional differentiation is used. As the permanent $|\vec{n}\rangle$ is constructed from repeatedly applying creation operators of particles in the M orbitals, it can be regarded to be given by multiple integrations over the orbitals $\phi_k(\vec{x})$,

$$|\vec{n}\rangle = \cdots \int \mathrm{d}\vec{x}_\alpha \phi_i(\vec{x}_\alpha)\hat{\Psi}^\dagger(\vec{x}_\alpha) \int \mathrm{d}\vec{x}_\beta \phi_j(\vec{x}_\beta)\hat{\Psi}^\dagger(\vec{x}_\beta)\cdots|\mathrm{vac}\rangle. \tag{45}$$

As each functional differentiation contributes to the result, this will be counted by a factor $\hat{a}_k^\dagger$, which results in $\frac{\partial\langle\Phi|}{\partial\phi_k^*(\vec{x})} = \langle\Phi|\hat{a}_k^\dagger\hat{\Psi}(\vec{x})$. But as the full hamiltonian $\hat{H}$, which is given in field form by Eq.(3), is independent on the M orbitals chosen, the functional differentiation of $\hat{H}$ with respect to the orbitals $\{\phi_k\}$ gives zero, $\frac{\partial\hat{H}}{\partial\phi_k^*(\vec{x})} = 0$. Then functional variation of $E_{G^\mathcal{M}}$ Eq. (40) with respect to the orbitals $\{\phi_k\}$, combined with the functional constraints Eq. (42), leads to

$$\frac{\partial E_{G^\mathcal{M}}}{\partial\phi_k^*(\vec{x})} = \Big[\sum_{\vec{m}\in\mathcal{M}}\langle\vec{m}|C_{\vec{m}}^*\Big]\hat{a}_k^\dagger\hat{\Psi}(\vec{x})\hat{H}\Big[\sum_{\vec{n}\in\mathcal{M}}C_{\vec{n}}|\vec{n}\rangle\Big] = \sum_{j=1}^{M}\lambda_{kj}\phi_j(\vec{x}), \tag{46}$$

where $\lambda_{jk} = \lambda_{kj}^*$ is Hermitian matrix. Here the method of Lagrange multipliers with complex functional variables is used. Integrating each side over space after multiplication with $\phi_l^*(\vec{x})$ yields

$$\Big[\sum_{\vec{m}\in\mathcal{M}}\langle\vec{m}|C_{\vec{m}}^*\Big]\hat{a}_k^\dagger\hat{a}_l\hat{H}\Big[\sum_{\vec{n}\in\mathcal{M}}C_{\vec{n}}|\vec{n}\rangle\Big] = \begin{cases}\lambda_{kl} & \text{for } l\leq M\\ 0 & \text{for } l > M.\end{cases} \tag{47}$$

Here, using Eq. (43) and the property that $\vec{m}_k^l \in \mathcal{M}$ when $k,l\leq M$ and $\vec{m}\in\mathcal{M}$, the undetermined set of Lagrange multipliers λ_{kl} becomes related to $E_{G^\mathcal{M}}$ by $\lambda_{kl} = E_{G^\mathcal{M}}\langle\hat{a}_{kl}^\dagger\rangle$ for $k,l\leq M$. Using Eq. (3) and the bosonic commutation relations between field operators, i.e. $[\hat{\Psi}(\vec{x}),\hat{\Psi}^\dagger(\vec{x}')] = \delta\big(\vec{x}-\vec{x}'\big)$, $[\hat{\Psi}(\vec{x}),\hat{a}_k^\dagger] = \phi_k(\vec{x})$, and so on, Eq. (46) $\langle\hat{a}_k^\dagger\hat{\Psi}(\vec{x})\hat{H}\rangle = \sum_{j=1}^M\lambda_{kj}\phi_j(\vec{x})$ is explicitly expressed as

$$\begin{aligned}&\sum_{j=1}^{\infty}\langle\hat{a}_{kj}^\dagger\rangle\Big[-\frac{\nabla^2}{2m}+V_{\mathrm{trap}}(\vec{x})\Big]\phi_j(\vec{x}) + \langle\hat{a}_k^\dagger\hat{H}\hat{\Psi}(\vec{x})\rangle\\ &+\sum_{p,q,j=1}^{\infty}\langle\hat{a}_{kpqj}^{\dagger\dagger}\rangle\int\mathrm{d}\vec{x}'\ \phi_p^*(\vec{x}')V(\vec{x},\vec{x}')\phi_q(\vec{x}')\phi_j(\vec{x}) = \sum_{j=1}^{M}\lambda_{kj}\phi_j(\vec{x}).\end{aligned} \tag{48}$$

Since we can eliminate the annihilations above M, we obtain

$$\begin{aligned}&\sum_{j=1}^{M}\langle\hat{a}_{kj}^\dagger\rangle\hat{h}\phi_j(\vec{x}) + \sum_{p,q,j=1}^{M}\langle\hat{a}_{kpqj}^{\dagger\dagger}\rangle\hat{V}_{pq}\phi_j(\vec{x}) = \sum_{j=1}^{M}\Big[\lambda_{kj}-\langle\hat{a}_k^\dagger\hat{H}\hat{a}_j\rangle\Big]\phi_j(\vec{x})\\ &= \sum_{j=1}^{M}\Big[E_{G^M}\langle\hat{a}_k^\dagger\hat{a}_j\rangle - \langle\hat{a}_k^\dagger\hat{H}\hat{a}_j\rangle\Big]\phi_j(\vec{x}) \equiv \sum_{j=1}^{M}\tilde{\lambda}_{kj}\phi_j(\vec{x}),\end{aligned} \tag{49}$$

where the new undetermined Lagrange multipliers $\tilde{\lambda}_{kj} \equiv \lambda_{kj} - \langle \hat{a}_k^\dagger \hat{H} \hat{a}_j \rangle$ which satisfy $\tilde{\lambda}_{kj}^* = \tilde{\lambda}_{jk}$ are introduced. We abbreviated, for the sake of convenience, two single-particle and interaction operators defined by

$$\hat{h}\phi_j(\vec{x}) \equiv \Big[-\frac{\nabla^2}{2m} + V_{\rm trap}(\vec{x}) \Big] \phi_j(\vec{x}) \tag{50}$$

and

$$\hat{V}_{pq}\phi_j(\vec{x}) \equiv \int \mathrm{d}\vec{x}' \ \phi_p^*(\vec{x}') V(\vec{x},\vec{x}') \phi_q(\vec{x}') \phi_j(\vec{x}). \tag{51}$$

4.2. Approaching the many-body state

To find the tentative ground state $|G^M\rangle$, we have to find the coefficient $C_{\vec{n}}$'s and the complex orbital functions $\phi_k(\vec{x})$ satisfying Eq. (44) and (49). Additionally, the solutions must satisfy all $(1 + M^2)$ constraints Eq. (41, 42). The number of real values which we should find is $2\frac{(N+M-1)!}{N!(M-1)!}$ for the set of the $C_{\vec{n}}$, $2M$ real functions for the $\phi_k(\vec{x})$, and $(1 + M^2)$ for the undetermined Lagrange multiplier E_{G^M} and the λ_{kj}. The number of given real equations therefore is $2\frac{(N+M-1)!}{N!(M-1)!}$ for Eq. (44), $2M$ real functional equations for Eq. (49), and $(1+M^2)$ for Eq. (41, 42). Apart from the large number of variables, what makes matters even more complicated is that the equations (41, 42, 44, 49) are coupled together. To find a self-consistent solution is therefore obviously a very difficult problem.

In ref. [17], the authors started from an initial guess, then iteratively, with a convergence check, they obtained a solution. A few years later in ref. [9], applying the Wick rotation $it \to \tau$ on the equations of motion, they introduced the so-called imaginary time propagation. They claimed that this reduces any arbitrary initial many-body state after a sufficient time of propagation to the ground state. The imaginary time evolution $i\frac{\partial}{\partial t}|\Phi\rangle = \hat{H}|\Phi\rangle \Rightarrow -\frac{\partial}{\partial \tau}|\Phi\rangle = \hat{H}|\Phi\rangle$ implies that $e^{-i\hat{H}t} \Rightarrow e^{-\hat{H}\tau}|\Phi\rangle$. As τ goes to infinity, this seems to indicate that only the ground state survives and the excited states would no longer contribute. The contribution of the excited states decays exponentially according to a factor which is proportional to energy difference from the ground state and τ.

Here, we present alternatively the method of steepest constrained descent described in section 3. This method of a approaching a minimum (maximum) from an initial trial state will guarantee that any given state is propagated to the neighboring lowest (highest) value point along the steepest path for given variational parameters. Though it propagates a state only to a local neighboring minimum (maximum) point, we can find in many cases the global minimum, or the ground state, from a well-chosen initial state, and with in addition well-chosen variational parameters. Although this does not deliver the state along the shortest path, the very large number of degrees of freedom on the choice of variational parameters or the sequential processing (separation) of variations can compensate it in many cases. The flexibility of this method will therefore be beneficial for finding the ground state.

Let us see the process in more detail. The first step is to find (by educated guess) an appropriate initial state, specifying the coefficients $C_{\vec{n}}$ and the M orbitals which we believe are appropriate to approximately describe the ground state of a given system. From this initial guess, the state is propagated as

follows. For the expansion coefficient $C_{\vec{n}}$'s, using Eq. (39),

$$\frac{dC_{\vec{n}}}{d\tau} = -\Delta_C(\tau)\Big[\langle\vec{n}|\hat{H}\sum_{\vec{m}} C_{\vec{m}}|\vec{m}\rangle - \lambda C_{\vec{n}},\Big] \tag{52}$$

where $\Delta_C(\tau)$ is any arbitrary positive function of τ which is introduced to satisfy $\sum_{\vec{n}} \frac{dC^*_{\vec{n}}}{d\tau}\frac{dC_{\vec{n}}}{d\tau} = \text{const}$ at a certain given instant τ and therefore can be chosen in a convenient way to save time and calculation costs. Since it must satisfy $\sum_{\vec{n}} C^*_{\vec{n}}C_{\vec{n}} = 1$, i.e. $\sum_{\vec{n}}\left[C^*_{\vec{n}}\frac{dC_{\vec{n}}}{d\tau} + \frac{dC^*_{\vec{n}}}{d\tau}C_{\vec{n}}\right] = 0$, where $\lambda = \langle\hat{H}\rangle$.

As another option, we can use a polar representation for $C_{\vec{n}}$. Representing the complex variable $C_{\vec{n}}$ by an Euler representation with a radius $\xi_{\vec{n}}$ and an angle $\theta_{\vec{n}}$ gives $C_{\vec{n}} = \xi_{\vec{n}}e^{i\theta_{\vec{n}}}$. Then the constraint Eq. (41) becomes $\sum_{\vec{n}}\xi^2_{\vec{n}} = 1$, restricting only the radial component of the complex variables $C_{\vec{n}}$. Since we do not have to confine the variable change into the specific form $\sum_{\vec{n}}\left[\left(\frac{d\xi_{\vec{n}}}{d\tau}\right)^2 + \xi^2_{\vec{n}}\left(\frac{d\theta_{\vec{n}}}{d\tau}\right)^2\right] = \text{const}$, separating the two variable sets can be much more efficient in this case. That is, we set $\frac{d\xi_{\vec{n}}}{d\tau} = 0$ and $\sum_{\vec{n}}\left(\frac{d\theta_{\vec{n}}}{d\tau}\right)^2 = \text{const}$ for some given τ time spans which would be chosen in computationally favorable way, and $\frac{d\theta_{\vec{n}}}{d\tau} = 0$ and $\sum_{\vec{n}}\left(\frac{d\xi_{\vec{n}}}{d\tau}\right)^2 = \text{const}$ for the other τ spans. Then the method of steepest constrained descent gives

$$\frac{d\xi_{\vec{n}}}{d\tau} = 0, \qquad \frac{d\theta_{\vec{n}}}{d\tau} = -\Delta_\theta(\tau)\Im\big(\xi_{\vec{n}}e^{-i\theta_{\vec{n}}}\langle\vec{n}|\hat{H}\rangle\big), \tag{53}$$

for some given τ spans, and

$$\frac{d\theta_{\vec{n}}}{d\tau} = 0, \qquad \frac{d\xi_{\vec{n}}}{d\tau} = -\Delta_\xi(\tau)\Big[\Re\big(e^{-i\theta_{\vec{n}}}\langle\vec{n}|\hat{H}\rangle\big) - \lambda\xi_{\vec{n}}\Big] \tag{54}$$

for the other following τ-intervals. Here $\Re$ means real part of complex number and $\Im$ means imaginary part of complex number. Using $\sum_{\vec{n}}\xi^2_{\vec{n}} = 1$, and therefore $\sum_{\vec{n}} 2\xi_{\vec{n}}\frac{d\xi_{\vec{n}}}{d\tau} = 0$, then λ becomes $\lambda = \langle\hat{H}\rangle$ too. Dealing with $\xi_{\vec{n}}$ and $\theta_{\vec{n}}$ separately, we propagate the two variable sets successively and iteratively until convergence is achieved. With any sequence, they will finally approach the minimum.

For the orbitals $\phi_k(\vec{x})$, the method of steepest constrained descent gives

$$\begin{aligned}\frac{d\phi_k(\vec{x})}{d\tau} &= -\Delta_{\phi_k}(\tau)\Big[\langle\hat{a}^\dagger_k\hat{\Psi}(\vec{x})\hat{H}\rangle - \sum_{j=1}^{M}\lambda_{kj}\phi_j(\vec{x})\Big] \\ &= -\Delta_{\phi_k}(\tau)\Big[\sum_{j=1}^{M}\langle\hat{a}^\dagger_{kj}\rangle\hat{h}\phi_j(\vec{x}) + \sum_{p,q,j=1}^{M}\langle\hat{a}^{\dagger\dagger}_{kpqj}\rangle\hat{V}_{pq}\phi_j(\vec{x}) - \sum_{j=1}^{M}\tilde{\lambda}_{kj}\phi_j(\vec{x})\Big].\end{aligned} \tag{55}$$

If we propagate the orbitals separately one after another, i.e. only the k-th orbital changes within a certain period, the constraint becomes $\int \mathrm{d}\vec{x}\ \phi^*_l(\vec{x})\frac{\phi_k(\vec{x})}{d\tau} = 0$ for $l \neq k$ and $\int \mathrm{d}\vec{x}\ \left(\phi^*_k(\vec{x})\frac{\phi_k(\vec{x})}{d\tau} + \frac{\phi^*_k(\vec{x})}{d\tau}\phi_k(\vec{x})\right) = 0$. Then the undetermined Lagrange multipliers becomes

$$\tilde{\lambda}_{kl} = \sum_{j=1}^{M}\langle\hat{a}^\dagger_{kj}\rangle\epsilon_{lj} + \sum_{p,q,j=1}^{M}\langle\hat{a}^{\dagger\dagger}_{kpqj}\rangle V_{lpqj} \tag{56}$$

and

$$\tilde{\lambda}_{kk} = \Re\Big(\sum_{j=1}^{M} \langle \hat{a}_{kj}^{\dagger} \rangle \epsilon_{kj} + \sum_{p,q,j=1}^{M} \langle \hat{a}_{kpqj}^{\dagger\dagger} \rangle V_{kpqj} \Big). \tag{57}$$

Separating the propagation of the orbitals, i.e. propagating the orbitals one after another independently, makes the process much easier and more comprehensible.

For the numerical implementation by computers, a discrete variable representation technique (commonly abbreviated DVR in the literature) will be used to represent the continuous orbital functions with a finite number of discrete variables [16]. Based on well-known orthonormal functions such as, e.g., the harmonic oscillator eigenfunctions, sinusoidal, Bessel, and Legendre polynomials, we can express any continuous function as

$$\phi_k(\vec{x}) = \sum_{\bar{l}=1}^{\infty} \zeta_{k\bar{l}} \phi_{\bar{l}}. \tag{58}$$

This is mathematically founded on the completeness of eigenfunctions and Sturm-Liouville theory. With an appropriate choice of the eigenfunction set, several hundreds of eigenfunctions will be sufficient to describe the continuous functions $\phi_k(\vec{x})$ [16, 18, 19, 20].

Then the change of orbitals will be expressed as

$$\frac{d\zeta_{k\bar{l}}}{d\tau} = -\Delta_{\phi_k}(\tau) \Bigg[\sum_{j=1}^{M} \langle \hat{a}_{kj}^{\dagger} \rangle \epsilon_{\bar{l}j} + \sum_{p,q,j=1}^{M} \langle \hat{a}_{kpqj}^{\dagger\dagger} \rangle V_{\bar{l}pqj} - \sum_{j=1}^{M} \tilde{\lambda}_{kj} \zeta_{j\bar{l}} \Bigg]. \tag{59}$$

With these successive and iterative propagation steps, we can approach the ultimate form of the ground state $|G^{\mathcal{M}}\rangle$ in the sub-Hilbert space.

5. Control of truncated many-body evolution

5.1. Evaluating the error of truncated many-body evolution

An instantaneous error is expressed by Eq. (21). Minimizing this error with a state change under the truncation Eq. (13) gives us the appropriate truncated many-body evolution. This offers, as a major benefit of the present approach, a quantitative value, the error, which indicates how accurately the truncated evolution describes the exact one.

Explicitly expressing the error, we have

$$\begin{aligned}
&\langle \Phi | \big[\hat{H} - i\partial_t \big]^{\dagger} \big[\hat{H} - i\partial_t \big] | \Phi \rangle \\
&= \sum_{\vec{n} \in \mathcal{M}(t)} \Bigg[\langle \vec{n} | C_{\vec{n}}^{*} \hat{H} + \langle \vec{n} | \big(i\partial_t C_{\vec{n}}^{*} \big) + \sum_{i=1}^{M} \langle \vec{n} | C_{\vec{n}}^{*} \hat{a}_i^{\dagger} \int \mathrm{d}\vec{x} \big(i\partial_t \phi_i^{*}(\vec{x}, t) \big) \hat{\Psi}(\vec{x}) \Bigg] \\
&\times \sum_{\vec{m} \in \mathcal{M}(t)} \Bigg[\hat{H} C_{\vec{m}} | \vec{m} \rangle - \big(i\partial_t C_{\vec{m}} \big) | \vec{m} \rangle - \sum_{j=1}^{M} \int \mathrm{d}\vec{x}' \big(i\partial_t \phi_j(\vec{x}', t) \big) \hat{\Psi}^{\dagger}(\vec{x}') \hat{a}_j C_{\vec{m}} | \vec{m} \rangle \Bigg].
\end{aligned} \tag{60}$$

We minimize this instantaneous error, varying the complex variables $\big(\partial_t C_{\vec{n}}\big)$ and $\big(\partial_t \phi_i(\vec{x},t)\big)$ subject to the $(1+M^2)$ constraints

$$\begin{aligned} &\partial_t\Big[\sum_{\vec{n}} C^*_{\vec{n}}(t)C_{\vec{n}}(t) = 1\Big] \\ &\Rightarrow \quad \sum_{\vec{n}}\Big[\big(\partial_t C^*_{\vec{n}}(t)\big)C_{\vec{n}}(t) + C^*_{\vec{n}}(t)\big(\partial_t C_{\vec{n}}(t)\big)\Big] = 0 \end{aligned} \tag{61}$$

and from the orthonormality condition

$$\begin{aligned} &\partial_t\Big[\int \mathrm{d}\vec{x}\phi^*_i(\vec{x},t)\phi_j(\vec{x},t) = \delta_{ij}\Big] \\ &\Rightarrow \quad \int \mathrm{d}\vec{x}\Big[\big(\partial_t\phi^*_i(\vec{x},t)\big)\phi_j(\vec{x},t) + \phi^*_i(\vec{x},t)\big(\partial_t\phi_j(\vec{x},t)\big)\Big] = 0. \end{aligned} \tag{62}$$

The Eq. (61) requires probability conservation of the state itself and Eq. (62) requires conservation of orthonormality of orbitals. Using the expression Eq. (17), Eq. (62) can be expressed as the hermiticity condition $t^*_{ji} = t_{ij}$.

Variation with respect to $\partial_t C^*_{\vec{n}}$ leads to

$$\langle\vec{n}|i\big[\hat{H} - i\partial_t\big]|\Phi\rangle = \lambda(t)C_{\vec{n}} \tag{63}$$

resulting in

$$i\partial_t C_{\vec{n}} = \langle\vec{n}|\big[\hat{H} - \sum_{i=1}^{\infty}\sum_{j=1}^{M} t_{ij}\hat{a}^\dagger_{ij}\big]|\Phi\rangle + i\lambda(t)C_{\vec{n}}. \tag{64}$$

As the constraint Eq. (61) enforces $\lambda(t) = 0$,

$$\langle\vec{n}|\big[\hat{H} - i\partial_t\big]|\Phi\rangle = 0, \tag{65}$$

and therefore the time evolution of the expansion coefficients takes the form

$$i\partial_t C_{\vec{n}} = \langle\vec{n}|\big[\hat{H} - \hat{t}\ \big]|\Phi\rangle \tag{66}$$

where $\vec{n} \in M(t)$ and $\hat{t} = \sum_{i,j} t_{ij}\hat{a}^\dagger_{ij}$.

Variation with respect to $\partial_t\phi^*_k(\vec{x},t)$ gives

$$\langle\Phi|i\hat{a}^\dagger_k\hat{\Psi}(\vec{x})\big[\hat{H} - i\partial_t\big]|\Phi\rangle = \sum_{l=1}^{M}\lambda_{kl}\phi_l(\vec{x},t). \tag{67}$$

After multiplying both sides with $\phi^*_l(\vec{x},t)$ and integrating, one finds

$$\langle\Phi|i\hat{a}^\dagger_k\hat{a}_l\big[\hat{H} - i\partial_t\big]|\Phi\rangle = \begin{cases}\lambda_{kl}(t) & \text{if } l \le M \\ 0 & \text{if } l > M.\end{cases} \tag{68}$$

Since $\langle\vec{n}|\hat{a}^\dagger_{kl}$ belongs to $\mathcal{M}(t)$ whenever $\vec{n} \in \mathcal{M}(t)$ and $k,l \le M$, all $\lambda_{kl}(t)$ here become zero too with the help of Eq. (65). So for any k and l,

$$\langle\Phi|\hat{a}^\dagger_{kl}\big[\hat{H} - i\partial_t\big]|\Phi\rangle = 0. \tag{69}$$

Expanding the above equation for $l > M$,

$$\langle \hat{a}_{kl}^\dagger \hat{H} \rangle = \sum_{j=1}^{M} \langle \hat{a}_{kj}^\dagger \rangle \int \mathrm{d}\vec{x} \phi_l^*(\vec{x},t) \big(i\partial_t \phi_j(\vec{x},t) \big). \tag{70}$$

Since the SPDM can be noninvertible, we reduce the density matrix by eliminating unoccupied orbitals in which the eigenvalues of the SPDM becomes zero (relative to $\mathcal{O}(N)$ in the limit $N \to \infty$) after diagonalizing the SPDM. In the process of diagonalizing the SPDM, the orbitals are unitarily transformed so that the essentially unoccupied orbitals can be found and eliminated. Introducing the inverse of this reduced density matrix $\langle \rho_{ki} \rangle \equiv \langle \hat{a}_{ki}^\dagger \rangle \equiv \langle \hat{a}_k^\dagger \hat{a}_i \rangle$ when the $\mathcal{O}(N)$ occupied orbitals exist up to the M_1th orbital ($\sum_{i=1}^{M_1} \langle \rho \rangle_{ki}^{-1} \langle \rho_{ij} \rangle = \delta_{kj}$) and using the completeness relation $\sum_{l=1}^{\infty} \phi_l^*(\vec{x}',t)\phi_l(\vec{x},t) = \delta(\vec{x}' - \vec{x})$, the evolution equation of the orbitals acquires the form

$$\begin{aligned}
i\partial_t \phi_k(\vec{x},t) &= \sum_{l=1}^{M} t_{lk} \phi_l(\vec{x},t) + \sum_{l=M+1}^{\infty} \sum_{i=1}^{M_1} \langle \rho \rangle_{ki}^{-1} \langle \hat{a}_i^\dagger \hat{a}_l \hat{H} \rangle \phi_l(\vec{x},t) \\
&= \sum_{l=1}^{M} t_{lk} \phi_l(\vec{x},t) + \sum_{l=M+1}^{\infty} \sum_{i=1}^{M_1} \langle \rho \rangle_{ki}^{-1} \Big\langle \Big[\sum_{n=1}^{M_1} \epsilon_{ln} \hat{a}_{in}^\dagger + \sum_{n,p,q=1}^{M_1} V_{lnpq} \hat{a}_{inpq}^{\dagger\dagger} \Big] \Big\rangle \phi_l(\vec{x},t) \\
&= \sum_{l=1}^{M} t_{lk} \phi_l(\vec{x},t) + \sum_{l=M+1}^{\infty} \Big[\epsilon_{lk} + \sum_{i,n,p,q=1}^{M_1} V_{lnpq} \langle \rho \rangle_{ki}^{-1} \langle \hat{a}_{inpq}^{\dagger\dagger} \rangle \Big] \phi_l(\vec{x},t)
\end{aligned} \tag{71}$$

for $k \leq M_1$.

Here, we divide the evolution of the orbitals into two parts. We call the left $l \leq M$ part of Eq. (71) inner rotation and the right $l > M$ part of Eq. (71) rotation toward the outside the sub-Hilbert space. Since the sub-Hilbert space spanned by M orbitals, $\sum_{i=1}^{M} c_i \phi_i(\vec{x},t)$, does not change under inner rotation, we realize that only a rotation toward the outside deforms the sub-Hilbert space. For the evolution inside the sub-Hilbert space, i.e. inner rotation, we simply use t_{ij} defined in (16), which can be any Hermitian matrix. Using Eq. (65, 69, 71), the expression for the error Eq. (60) can be strongly simplified:

$$\begin{aligned}
&\langle \Phi | \big[\hat{H} - i\partial_t \big]^\dagger \big[\hat{H} - i\partial_t \big] | \Phi \rangle = \langle \Phi | \big[\frac{1}{2} \sum_{i,j,k,l=1}^{\infty} V_{ijkl} \hat{a}_{ijkl}^{\dagger\dagger} \big] \big[\hat{H} - i\partial_t \big] | \Phi \rangle \\
&= \frac{1}{2} \sum_{i,j=1}^{M_1} \sum_{k,j=1}^{\infty} V_{ijkl} \langle \Phi | \hat{a}_{ijkl}^{\dagger\dagger} \big[\hat{H} - i\partial_t \big] | \Phi \rangle \\
&= - \sum_{i,j,k,n,r,s,p,q=1}^{M_1} \sum_{l=M+1}^{\infty} V_{ijkl} V_{lspq} \langle \hat{a}_{ijkn}^{\dagger\dagger} \rangle \langle \rho \rangle_{nr}^{-1} \langle \hat{a}_{rspq}^{\dagger\dagger} \rangle \\
&\quad + \sum_{i,j,p,q=1}^{M_1} \sum_{k,s=1}^{M} \sum_{l=M+1}^{\infty} V_{ijkl} V_{lspq} \langle \hat{a}_{ijk}^{\dagger\dagger} \hat{a}_{spq}^\dagger \rangle + \frac{1}{2} \sum_{i,j,p,q=1}^{M_1} \sum_{k,l=M+1}^{\infty} V_{ijkl} V_{lkpq} \langle \hat{a}_{ijpq}^{\dagger\dagger} \rangle.
\end{aligned} \tag{72}$$

The above equation represents our main result, rendering the error of many-body quantum evolution upon truncation systematically computable. As clearly

seen, the error stems entirely from interactions. In other words, the error does not depend on the choice of t_{ij} and even on the single particle energy matrix ϵ_{ij} for any given truncated initial state, provided the evolution of the state, $\partial_t|\Phi\rangle$, is optimally taken as in Eq. (65, 69, 71).

5.2. Determining the number of orbitals dynamically

When the error becomes large or, alternatively, when we aim at describing the system more precisely, we have to increase the number of orbitals M_1 into M. The $(M - M_1)$ additional orbitals then can be determined by variation of the error with respect to $\phi_u(\vec{x}, t)$ where $M_1 < u \leq M$, and subject to the orthonormalization condition $\int \mathrm{d}\vec{x}\ \phi_u^*(\vec{x}, t)\phi_v(\vec{x}, t) = \delta_{uv}$. The method of Lagrange multipliers for functional variables gives the stationary condition

$$\begin{aligned}&\sum_{i,j,k,n,r,s,p,q=1}^{M_1} V_{ijku}\big(\hat{V}_{sp}\phi_q(\vec{x}, t)\big)\langle\hat{a}^{\dagger\dagger}_{ijkn}\rangle\langle\rho\rangle^{-1}_{nr}\langle\hat{a}^{\dagger\dagger}_{rspq}\rangle \\ &- \sum_{i,j,p,q=1}^{M_1}\sum_{k,s=1}^{M} V_{ijku}\big(\hat{V}_{sp}\phi_q(\vec{x}, t)\big)\langle\hat{a}^{\dagger\dagger}_{ijk}\hat{a}^{\dagger}_{spq}\rangle = \sum_{v=1}^{M}\mu_{uv}\phi_v(\vec{x}, t).\end{aligned} \tag{73}$$

While this is an equation for the additional orbitals, the additional orbitals are difficult to obtain directly from the above equation. As mentioned already in section 3.2, the best we can do is to guess some orbitals that will approximately satisfy the above equation.

Therefore, we use the method of steepest constrained descent again. From an initial trial orbital, we propagate the orbital toward

$$\begin{aligned}\frac{d\phi_u(\vec{x})}{d\tau} = -\Delta_{\phi_u}(\tau)\Bigg[&\sum_{i,j,k,n,r,s,p,q=1}^{M_1} V_{ijku}\big(\hat{V}_{sp}\phi_q(\vec{x}, t)\big)\langle\hat{a}^{\dagger\dagger}_{ijkn}\rangle\langle\rho\rangle^{-1}_{nr}\langle\hat{a}^{\dagger\dagger}_{rspq}\rangle \\ &- \sum_{i,j,p,q=1}^{M_1}\sum_{k,s=1}^{M} V_{ijku}\big(\hat{V}_{sp}\phi_q(\vec{x}, t)\big)\langle\hat{a}^{\dagger\dagger}_{ijk}\hat{a}^{\dagger}_{spq}\rangle - \sum_{v=1}^{M}\mu_{uv}\phi_v(\vec{x}, t)\Bigg]\end{aligned} \tag{74}$$

so that the error become minimized with this additional orbital. If we propagate orbitals separately and iteratively one after another, i.e. only the uth orbital changes along τ, the constraint becomes $\int \mathrm{d}\vec{x}\ \phi_v^*(\vec{x})\frac{\phi_u(\vec{x})}{d\tau} = 0$ for $v \neq u$ and $\int \mathrm{d}\vec{x}\ \left(\phi_u^*(\vec{x})\frac{\phi_u(\vec{x})}{d\tau} + \frac{\phi_u^*(\vec{x})}{d\tau}\phi_u(\vec{x})\right) = 0$. Then the undetermined Lagrange multipliers become

$$\begin{aligned}\mu_{uv} = &\sum_{i,j,k,n,r,s,p,q=1}^{M_1} V_{ijku}V_{vspq}\langle\hat{a}^{\dagger\dagger}_{ijkn}\rangle\langle\rho\rangle^{-1}_{nr}\langle\hat{a}^{\dagger\dagger}_{rspq}\rangle \\ &- \sum_{i,j,p,q=1}^{M_1}\sum_{k,s=1}^{M} V_{ijku}V_{vspq}\langle\hat{a}^{\dagger\dagger}_{ijk}\hat{a}^{\dagger}_{spq}\rangle,\end{aligned} \tag{75}$$

where the orbital index rangea are constrained to be $M_1 < u \leq M$ and $1 \leq v \leq M$.

Since the inner rotation can be arbitrarily chosen, we can take the unit matrix, $t_{ij} = \epsilon_{ij}$, which renders the result in a simple form. The evolution

Eq. (66) for the expansion coefficients becomes

$$i\partial_t C_{\vec{n}} = \langle \vec{n}| \frac{1}{2} \sum_{i,j=1}^{M} \sum_{k,l=1}^{M_1} V_{ijkl} \hat{a}^{\dagger\dagger}_{ijkl} |\Phi\rangle \,. \tag{76}$$

This implies the desired property that, when the interaction is turned off, the coefficients $C_{\vec{n}}$ do not change at all. The Schrödinger equation for the orbitals, Eq. (71), becomes

$$i\partial_t \phi_k(\vec{x},t) = \hat{h}\phi_k(\vec{x},t) + \sum_{l=M+1}^{\infty} \sum_{i,n,p,q=1}^{M_1} V_{lnpq} \langle\rho\rangle^{-1}_{ki} \langle \hat{a}^{\dagger\dagger}_{inpq}\rangle \phi_l(\vec{x},t) \tag{77}$$

for $k \leq M_1$. The projection toward the outside of the sub-Hilbert space $\mathcal{M}$ takes place only on the interaction term. Thus the option of taking $t_{ij} = \epsilon_{ij}$ for the inner rotation shows the effect of the interaction term in this explicit manner.

For $M_1 < k \leq M$, the evolution of the additional orbitals can be chosen in any convenient way, since the time derivatives of the additional orbitals do not occur in the error measure. The only constraint is the inner rotation. As we have chosen $t_{lk}\big(\equiv \int \mathrm{d}\vec{x} \phi^*_l(\vec{x},t) i\partial_t \phi_k(\vec{x},t)\big)$ for $M_1 < l \leq M$ and $k \leq M_1$ to be ϵ_{lk}, t_{kl} should be $t^*_{lk} = \epsilon^*_{lk} = \epsilon_{kl}$ to satisfy the orthonormality constraint Eq. (62). Taking the rotation toward the outside of the sub-Hilbert space to be also equal to the single-particle energy matrix, ϵ_{kl} for $k > M$, the evolution of the additional orbital $\phi_l(\vec{x},t)$ for $M_1 < l \leq M$ is determined by the simple equation

$$i\partial_t \phi_l(\vec{x},t) = \hat{h}\phi_l(\vec{x},t), \tag{78}$$

while the additional orbitals are found from Eq. (74).

We, finally, emphasize again that the key difference from the MCTDHB approach is that additional macroscopically occupied orbitals during dynamical evolution can be found in our approach. By this means, we can handle the exceptional case when the SPDM is not invertible, and increase the number of orbitals under any given circumstances and boundary conditions.

6. Summary

Using McLachlan's principle, which is physically intuitive and simple, and the methods of Lagrange multiplication and steepest constrained descent, we have found a computationally feasible way to describe the many-body evolution of bosons in a rigorously controlled manner. Writing the many-body state in Hartree form and limiting the size of the Hilbert space by truncating into a finite number of macroscopically occupied field operator modes, the error from the exact evolution can be minimized self-consistently. This gives a variationally optimized solution to the evolution of the truncated many-body state.

We have demonstrated that without two-body interactions, our scheme possesses the desired property that the evolution of the many-body state can be exactly described with zero error, cf. Eq. (72). When interactions are turned on, the error accumulates during time evolution. Employing our method, we can evolve the truncated many-body state in an optimized way. Monitoring the error simultaneously, we can increase the accuracy of the evolution by increasing

the number of orbitals in a self-consistent way. By adaptively changing the number of orbitals based on the instantaneous error measure, we can automatically ensure the validity of the result for the many-body state.

We conclude by a brief summary of our approach applied to the well-known and ubiquitous Gross-Pitaevskiĭ equation. We start by evolving the initial trial state $|\Phi\rangle$ along the $M = 1$ version of Eq. (76, 77) and simultaneously check whether the error Eq. (72) remains small or not. Monitoring the error Eq. (72), we can determine under which conditions the Gross-Pitaevskiĭ equation loses its validity. When this happens, the error becoming large, we increase the number of orbitals to $M = 2$ (thus, here, $M_1 = 1$ and $M = 2$). The additional second orbital is found by the method of steepest constrained descent, using Eq. (74). Then the subsequent evolution of the quantum many-body state follows the $M = 2$ version of Eq. (76, 77), while the evolution of the (initially singular) second orbital follows Eq. (78). We monitor the error Eq. (72) again, checking that the error is decreased to a sufficient degree. In a self-consistent manner the processes described are carried out successively until we obtain a prescribed accuracy.

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References

[1] M. H. Anderson *et al.*, Science **269**, 198 (1995); K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995); C. C. Bradley, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. **78**, 985 (1997).

[2] For an overview, see *Ultracold Bosonic and Fermionic Gases*, Eds. K. Levin, A. L. Fetter and D. M. Stamper-Kurn, Contemporary Concepts of Condensed Matter Science Vol. 5, Elsevier, 2012.

[3] F. Dalfovo, S. Giorgini, L. P. Pitaevskiĭ, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).

[4] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).

[5] P. A. M. Dirac, Proc. Cambridge Philos. Soc. **26**, 376 (1930).

[6] J. Frenkel, *Wave Mechanics*, Clarendon Press, Oxford, 1934.

[7] A. D. McLachlan, Mol. Phys. **8**, 39 (2006).

[8] J. Broeckhove, L. Lathouwers, E. Kesteloot, and P. Van Leuven, Chem. Phys. Lett. **149**, 547 (1988).

[9] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. A. **77**, 033613 (2008).

[10] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. **100**, 130401 (2008).

[11] P. Bader and U. R. Fischer, Phys. Rev. Lett. **103**, 060402 (2009).

[12] K. Sakmann, A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. **103**, 220601 (2009).

[13] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. **106**, 240401 (2011).

[14] A. Raab, Chem. Phys. Lett. **319**, 674 (2000).

[15] H.-J. Kull and D. Pfirsch, Phys. Rev. E **61**, 5940 (2000).

[16] Z. Bacić and J. C. Light, J. Chem. Phys. **85**, 4594 (1986).

[17] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A. **73**, 063626 (2006).

[18] J. V. Lill, G. A. Parker, and J. C. Light, Chem. Phys. Lett. **89**, 483 (1982).

[19] J. C. Light, I. P. Hamilton, and J. V. Lill, J. Chem. Phys. **82**, 1400 (1985).

[20] N. Balakrishnan, C. Kalyanaraman, and N. Sathyamurthy, Phys. Rep. **280**, 79 (1997).